

High-Resolution Infrared Spectroscopy of Protoplanetary Disks

John S. Carr

Naval Research Laboratory, Washington, DC 20375, USA

Abstract. High-resolution spectroscopy at near and mid-infrared wavelengths can provide important and unique information about protoplanetary disks around young stars. In particular, infrared molecular spectroscopy is a good diagnostic of gas in the planet-forming regions of disks within ~ 10 AU of the star. Data on the physical conditions, gas content, structure, and chemistry of inner disks can be obtained through the analysis of velocity-resolved line profiles.

1 Introduction

1.1 Protoplanetary Disks and the Infrared

Planets are widely believed to form within protoplanetary accretion disks that are themselves a byproduct of the star formation process. Research has shown that circumstellar disks with the potential to form planets are very common around solar-mass stars of a few million years or less, implying that planetary systems could be common in the Galaxy. Indeed, the discovery of more than 100 extra-solar giant planets does demonstrate that planet formation is not a rare event. Planet searches have also revealed that giant planets have a remarkable range in mass and orbital characteristics, showing that planet formation can produce planetary systems very different from our Solar System. Hence, planet formation theory must not only explain the origin of the Solar System but must also account for the diversity of extra-solar planetary systems. In order to develop insight into the planet formation process, it is necessary to turn to observations of the planet-forming environments in circumstellar disks and to develop an understanding of the physical conditions in and evolution of protoplanetary disks around young stars.

Figure 1 provides a schematic of a protoplanetary disk around a classical T Tauri star. The classical T Tauri stars (CTTSs) are roughly one solar mass or less pre-main-sequence stars that are accreting material from their surrounding accretion disk. The generally accepted picture for CTTSs is illustrated in Fig. 1, in which the inner disk is truncated at several stellar radii by strong stellar magnetic fields, and material accretes onto the star along magnetic flux tubes. The disks themselves are relatively cool and optically thick in dust at most radii, producing the infrared excesses that are characteristic of CTTSs.

The inner regions of these accretion disks, within ~ 10 AU of the star, are of greatest relevance to the formation of planetary systems. At these radial distances are located Jupiter, Saturn, and the terrestrial planets in the Solar

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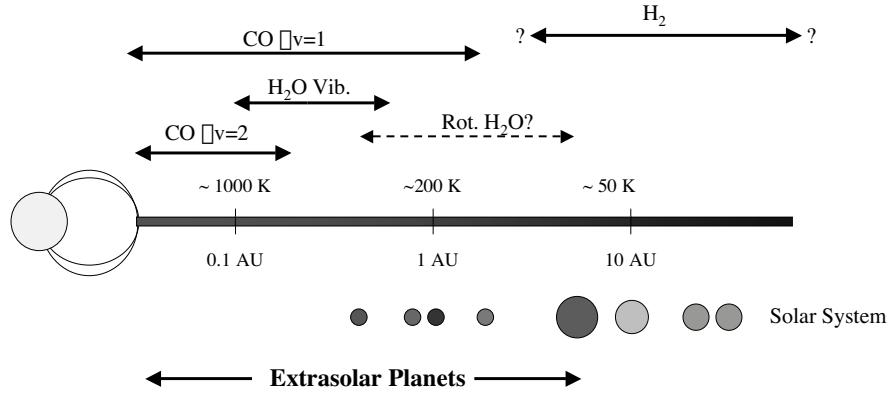


Fig. 1. A schematic of a protoplanetary accretion disk around a classical T Tauri star is shown with respect to the radial location of planets in the Solar System and known extra-solar planets. Approximate dust continuum temperatures are indicated at fiducial radii. At a radius of several stellar radii, the disk is truncated by a stellar magnetosphere, and material accretes onto the star along the field lines. The approximate radial locations of emission line diagnostics discussed in the text are shown.

System; all extra-solar planets discovered to date are located at radial distances from their stars of 0.04 to 3 AU. Because the effective temperatures of the disk at these radii fall in the range of ~ 100 K to ~ 1000 K, the Planck function peaks in the near to mid-infrared. These temperatures are low enough that the gas is molecular, except in the innermost disk where temperatures may reach a few 1000 K. However, the temperatures within several AU of the star are sufficiently high that the rotational and ro-vibrational levels of many molecules are excited. The ro-vibrational transitions for most molecules, and rotational transitions for a few key molecules, fall in the near and mid-infrared spectral regions. A large number of these spectral diagnostics are accessible with ground-based telescopes.

1.2 High-Resolution Spectroscopy

While the near to mid-infrared is clearly vital to the study of planet forming regions in disks, infrared spectroscopy at high-resolution becomes an indispensable tool for the study of the *gas component* of disks. Low-resolution is ideal for spectroscopy of the broad spectral features due to dust or ices, and some molecular bands and lines can be detected at low-resolution. However, high-resolution enables one to study the gas in inner disks in ways that are difficult or impossible to do at low-resolution. Because individual molecular transitions can be isolated and measured, it becomes easy to analyze the spectrum to derive gas temperatures, column densities, and relative abundances. The detection of very

weak lines is also enhanced at high-resolution. This is particularly important in searching for molecular species that may have very low abundances but which are of special interest to the study of protoplanetary disk chemistry. However, the prime advantage of high spectral resolution is the ability to obtain kinematic information from velocity-resolved line profiles. This can be especially powerful for disks in Keplerian rotation. If the inclination and stellar mass for the star-disk system are known, then for an ideal disk profile it is possible to determine the physical radii at which the spectral line is formed. When multiple transitions and molecular species are measured, the spectra can be analyzed to determine gas properties (temperature, column density, relative abundances) as a function of disk radius.

Spectral lines, either in emission or absorption, might be detected from disks under various circumstances. Four possible scenarios are illustrated in Fig. 2. For a typical CTTS, the accretion disk is optically thick in the continuum. If the surface layers of this disk are heated by some mechanism (e.g., radiation from the star), a temperature inversion may form in the upper atmosphere, and emission lines can be observed against the cooler continuum emission. Emission lines may also form in optically thin portions of a disk. For example, the disk could have an optically thin inner hole due to agglomeration of the dust, or a gap formed through the tidal influence of a stellar or giant protoplanetary companion. Gas remaining in these optically thin regions can form emission lines. In the extreme case that the entire disk is optically thin, spectral lines can trace the amount of residual disk gas.

Absorption lines could form in a disk if the vertical temperature profile decreases with disk height, similar to a stellar atmosphere. This is the situation for FU Orionis objects, very young stars in which the disk accretion rate is high enough that the accretion disk luminosity dominates the system. In FU Orionis stars, the inner disk is hot and dust free, and disk absorption profiles are observed in atomic and molecular transitions in both the infrared and optical [17]. For favorable geometries, absorption lines could also be formed in the cool, outer regions of a flared disk against the light of the star and inner disk. These special situations would give an opportunity to probe the outermost cold regions of the disk by a method that could complement millimeter-wave observations.

High-resolution infrared spectroscopy provides a powerful means to probe the gas in the inner planet-forming regions of protoplanetary disks. Some of the particular issues that infrared molecular spectroscopy can address include the radial and vertical structure of the disk, the gas content, gas dissipation timescales, molecular abundances, and protoplanetary disk chemistry. In this overview, examples of molecular *emission* lines observed in circumstellar disks around lower mass young stars will be discussed, and a few interesting results will be pointed out. The diagnostics that will be covered are indicated in Fig. 1 by their approximate radial locations in the disk.

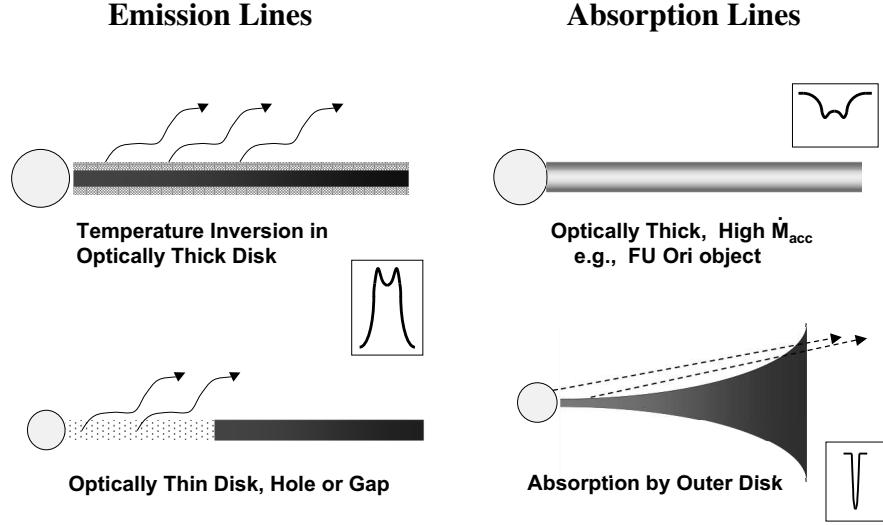


Fig. 2. Scenarios for the formation of spectral lines from protoplanetary accretion disks. Upper left: emission lines from a temperature inversion in the upper atmosphere of an optically thick disk. Lower left: emission lines from an optically thin disk, inner hole, or disk gap. Upper right: absorption lines formed in an optically thick disk atmosphere. Lower right: absorption lines formed in the cool outer regions of a flared disk against the light of the star or inner disk.

2 CO Overtone Emission

The first overtone bands of the CO molecule are the longest studied example of molecular emission from the disks of young stellar objects [9, 14, 27]. CO overtone emission is observed as a series of ro-vibrational bandheads from about 2.3 to 2.5 μm . The excitation of emission from these high rotational and vibrational levels requires the presence of hot gas ($> 2000 \text{ K}$) and rather high densities ($> 10^{10} \text{ cm}^{-3}$). Both low and high mass young stellar objects show CO overtone emission, but it is detected in only a few percent of young stars, typically objects that are most active or have the highest accretion rates.

High-resolution spectroscopy of CO bandhead emission in most young stars reveals the clear signature of a disk rotational profile [11, 13, 23]. The panels in Fig. 3 show how the numerous ro-vibrational transitions of the $v=2-0$ bandhead, when convolved with a double-peaked disk profile, produce a characteristic shape to the bandhead: a blue wing and shoulder, and an emission peak to the red of the bandhead center. The overtone emission most likely arises in the heated upper atmosphere of the disk [8]. The fitting of disk models to the CO bandheads in

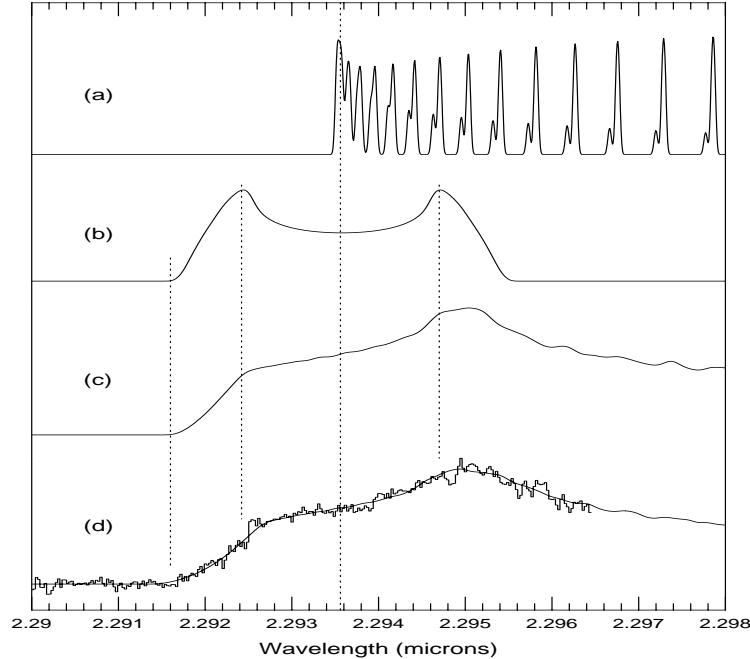


Fig. 3. Formation of the characteristic shape of the CO overtone bandhead due to emission from a disk in Keplerian rotation. Panel (a) shows the ro-vibrational transitions of the $v=2-0$ bandhead. The double-peaked profile for a single emission line from a rapidly rotating disk is shown in panel (b), and the convolution of this profile with the intrinsic CO spectrum is shown in (c). In panel (d), the model is compared to the observed spectrum of the young stellar object WL 16 [11].

low mass stars shows that the emission originates within a few tenths of an AU of the star, often extending to within a few stellar radii [11, 12, 23]. Hence, CO overtone emission probes the innermost radii of disks around low-mass young stars.

The CO transitions are closely spaced at the bandhead; this fact makes the shape of the bandhead very sensitive to the line optical depth and the *local* line broadening, and it is possible to separate the effects of the local line profile and the larger rotational profile. One interesting result from modeling of the CO bandheads is that very broad local profiles are usually required to fit the spectra [23], with velocity widths sometimes on the order of the sound speed [12]. If this line broadening is due to turbulence in the disk atmosphere, it may be associated with the viscosity that is responsible for angular momentum transport in the disk. Hence, more detailed study of the magnitude and shape of the local line broadening from disk emission lines may provide insights into this very fundamental aspect of protoplanetary accretion disks.

3 H₂O Emission

Water is another molecule that should be abundant in the gas phase in the inner regions of protoplanetary disks, at temperatures above the water-ice sublimation temperature (≈ 150 K) and below the dissociation temperature (≈ 2500 K). In many stars in which CO overtone emission is present, near-infrared ro-vibrational transitions of water have also been observed [12, 22]. Two examples are shown in Fig. 4. Analysis of the H₂O spectrum shows that the emission originates in hot gas with a characteristic excitation temperature of ≈ 1500 K. This is significantly lower than the characteristic temperature for the CO overtone emission (≥ 2500 K). In addition, in a given source the velocity widths of the H₂O emission lines are narrower than those of the CO overtone emission. Because H₂O dissociates at ~ 2500 K, compared to about 4000 K for CO, water emission should form at larger average radii than the CO emission. Hence, these results are consistent with a differentially rotating disk in which the atmospheric temperature decreases with increasing radius.

One interesting result is the abundance of H₂O that comes from jointly modeling the CO overtone and H₂O emission. The H₂O abundance relative to CO is found to be low, by factors of 2–10, compared to the expected abundance if the gas was in chemical equilibrium [12]. This may indicate that the abundances are controlled by physical processes other than equilibrium chemistry. In the upper disk atmosphere, photodissociation from UV photons is likely to be important, and strong Ly alpha emission could preferentially destroy some molecules, such as H₂O, compared to CO [5]. The energetic X-rays emitted by T Tauri stars are a major source of ionization in the disk atmosphere [16, 20] that directly affect the chemical abundances [1, 2, 15].

A disk atmosphere that has a significant thermal and chemical vertical structure is another factor that could alter the interpretation of the relative emission strengths. For example, modeling by [15] shows that X-ray induced heating and chemistry in the inner disk can produce a temperature inversion in the gas with a strong vertical gradient in the chemical abundances. The modeling of the H₂O and CO emission in [12] assumed a uniform vertical structure for the upper disk atmosphere. An apparent low abundance of H₂O could then arise if CO is actually present over a larger vertical column than H₂O, with H₂O found at larger depths and lower temperatures in the disk atmosphere. The addition of some non-equilibrium grain opacity to the H₂O line formation regions could further reduce the H₂O emission strengths.

This example highlights the prospects for studying chemistry in the inner regions of protoplanetary disks using infrared molecular spectroscopy. However, the above caveats also make it clear that physical models which calculate both the radial and vertical structure of the atmosphere may be needed in order to convert observed spectra into relative abundances.

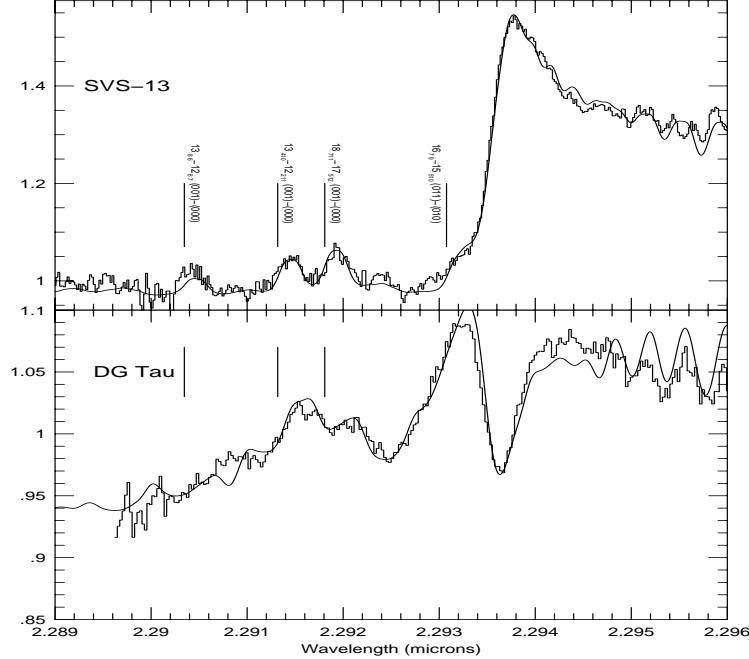


Fig. 4. Hot H₂O emission in the young stellar object SVS-13 and the classical T Tauri star DG Tau. The histograms are the observed spectra, and the smooth lines are disk models of the spectra. In SVS-13, the molecular emission is relatively narrow, and individual ro-vibrational transitions of H₂O can be resolved; identified transitions are labeled. Emission from the CO $v=2-0$ bandhead is seen at wavelengths longer than $\sim 2.2934\mu\text{m}$. In DG Tau, the H₂O emission lines are blended due to the rotational broadening; the double-peaked profile is most evident at $\approx 2.2918\mu\text{m}$. The dip in the CO bandhead at $\sim 2.2936\mu\text{m}$ is caused by CO absorption in the late-type stellar photosphere of DG Tau.

4 CO Fundamental Emission

The CO molecule has its fundamental ro-vibrational bands near $4.9\ \mu\text{m}$. The fundamental bands are sensitive to far smaller amounts of gas than the $2.3\ \mu\text{m}$ overtone bands, because the transitions probabilities are ~ 2 orders of magnitude greater. In addition, CO fundamental emission can be excited in cooler gas than the overtone, since emission can originate from the lower, first vibrational level. CO fundamental emission is detected in both CTTSs [10, 24] and intermediate mass Herbig Ae/Be stars [6, 7]. Lines from the $v=1-0$ and $2-1$ bands are commonly observed, and higher vibrational transitions and ^{13}CO lines have also been detected in some stars. Excitation by UV radiation may play a role in some Herbig Ae/Be stars [7].

Most of the classical T Tauri stars that have been observed show CO fundamental emission, in contrast to CO overtone emission, which is detected in very

few CTTSs. This difference in detection frequency reflects the more extreme conditions (higher temperatures and column densities) required to produce overtone emission. The derived excitation temperatures are in the range of 600–1800 K. In stars in which CO overtone emission is also present, however, the temperatures are ≈ 3000 K, consistent with analyses of the overtone emission. The strength of the CO fundamental emission (and excitation temperature, to a lesser extent) is correlated with indicators of the accretion rate. Assuming Keplerian rotation, the line profiles require that the CO emission extends over a large range in radii, from ~ 0.04 AU to at least 1 AU from the star.

CO fundamental emission in CTTSs is observed from single stars, wide binaries, and spectroscopic binaries [10, 24]. In single stars and wide binaries, the emission is likely to arise from a heated upper atmosphere of the optically thick accretion disk. The single star V836 Tau has properties that are intermediate between a CTTS and a weak-line T Tauri star, with an infrared spectral energy distribution that indicates the disk has an optically-thin inner hole. Weak CO emission is detected with velocity widths that place the gas within the hole. In the spectroscopic binary (SB) CTTSs, tidal disruption of the accretion disk is expected to produce a gap at radii centered on the stellar separation. In the two short-period SBs that have been studied, the CO emission profiles require that the emitting gas resides in the gap in the accretion disk, i.e., the gap is not totally empty of material. On the other hand, the CO emission profile in GW Ori, a long-period SB, indicates a *lack* of emission at radii near the expected disk gap. Hence, CO fundamental emission may be produced from disk atmospheres, gaps, and holes under different circumstances, and provides a probe of the structure of the inner disk.

The innermost radius for CO emission in CTTSs is one of the more interesting results from observations of the fundamental band. If the stellar mass and system inclination are known, then the maximum observed CO velocity gives the minimum radius for the CO emission if the gas is in Keplerian rotation. Since CO survives to rather high temperatures (4000–5000 K), the CO emission is likely to trace the inner radius of the disk. Figure 5 compares the inner CO radius to the corotation radius, where the angular velocity in the disk is equal to that of the star. The inner disk radius is relevant to magnetospheric accretion theories, and truncation of the disk (Fig. 1) is predicted to occur near the corotation radius. The plot shows that the inner CO radius is up to a factor of two inside of the corotation radius. Figure 5 also shows the distribution of orbital radii for known extra-solar giant planets (ExSGPs). The typical value for the inner disk radius as measured by CO is ≈ 0.04 AU, the same as the minimum radius at which short-period ExSGPs are observed to pile up. This coincidence strongly suggests that the disk plays a role in setting the minimum orbital radii of giant ExSGPs [21].

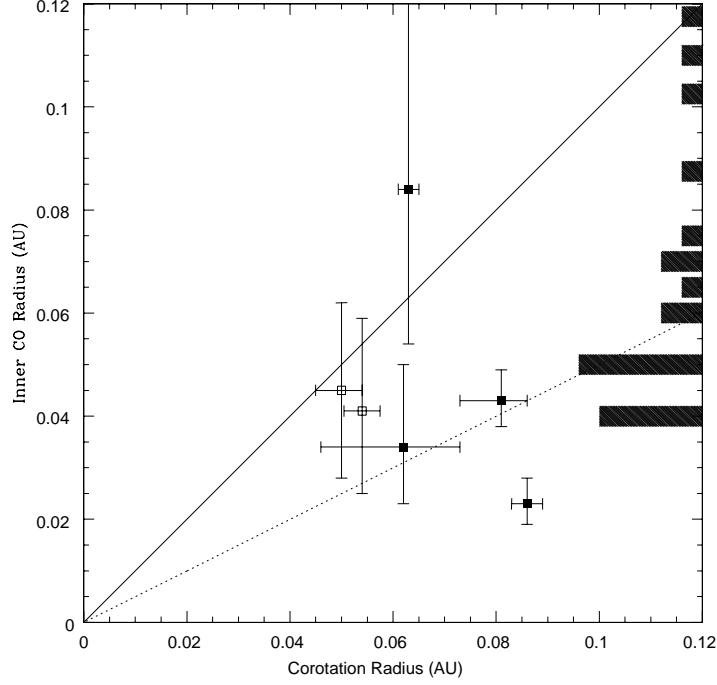


Fig. 5. Comparison of the inner CO emission radius and the corotation radius for single stars with known inclination and stellar mass [24]. The histogram on the right vertical axis shows the distribution of orbital radii for short-period extra-solar planets. The pile-up in orbital radii at ~ 0.04 AU is the same as the mean inner CO radius. The solid and dotted lines indicate an inner CO radius equal to 1.0 and 0.5 times the corotation radius, respectively.

5 Molecular Hydrogen

Molecular hydrogen is a key molecule to observe due to the fact that most of the mass in a protoplanetary disk resides in H₂. However, H₂ from protoplanetary disks has not been particularly easy to detect. Molecular hydrogen can be measured in three ways, the pure rotational transitions in the mid-infrared, the ro-vibrational transitions in the near-infrared, and the electronic bands in the UV [18, 19].

Both the near-infrared and mid-infrared lines of H₂ can be excited in gas at some distance from the star by shocks or ultraviolet radiation. Hence, it is important to rule out the possibility that detected H₂ emission arises from diffuse gas not associated with a disk. Velocity resolved line profiles and good spatial resolution are necessary for restricting the origin of the emission; line ratios of key transitions can help to determine the excitation mechanism for the emission.

The three lowest rotational lines of H₂ that can be observed from the ground are the S(1), S(2) and S(4) transitions at 17, 12 and 8 μm , respectively. These transitions can measure thermal emission from gas at temperatures ≥ 100 K and, being optically thin, should provide a direct measure of the gas mass. In the few young stars in which H₂ has been detected using high-resolution ground-based spectroscopy, the lines are $\leq 10 \text{ km s}^{-1}$ wide [25, 26], which indicates radii ~ 10 AU if the emission comes from a disk. An interesting puzzle, however, is the inability of high-resolution ground-based observations to confirm measurements of H₂ made by the Infrared Space Observatory [25, 28]. It is important to understand the reason for this discrepancy, because of the implications for the evolution of gas content in disks. This is relevant not only for the previous ISO results but also for upcoming Spitzer Space Telescope observations of H₂.

Thermal emission from the near-infrared ro-vibrational transitions of H₂ arises from hotter gas, ≥ 1000 K, but the transitions can also be excited in cooler gas by UV fluorescence or X-rays. The 2.12 μm 1-0 S(1) line has been detected in several CTTSs and WTTSs [3, 4], but it is not yet clear why particular stars show emission while others do not. Because transitions other than the 1-0 S(1) line have not been measured, the excitation mechanism has not been clearly identified. The detected lines are fairly narrow ($\approx 10 \text{ km/s}$), similar to the pure rotational H₂ lines. The linewidths, and the fact that T Tauri stars are sources of X-ray and ultraviolet radiation, suggest the possibility of radiative excitation of gas at several AU in the disk. Observations of H₂ in the far-ultraviolet are relevant in this context. Analysis of the far-UV H₂ spectrum in some CTTSs show Lyman-alpha pumping of H₂ emission and also reveal the presence of a thin, warm (~ 2500 K) disk surface layer at a few AU from the star [18, 19].

Summary

I have discussed some of the molecular emission features observed in the near and mid-infrared that are believed to probe the inner several AU of protoplanetary disks. These examples illustrate the potential for high-resolution infrared spectroscopy to provide unique information on the structure, gas content, and chemistry of protoplanetary disks at radii relevant to planet formation. New high-resolution infrared spectrographs planned for large telescopes will provide increased opportunities to make use of these diagnostics to increase our understanding of the origin of planetary systems.

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